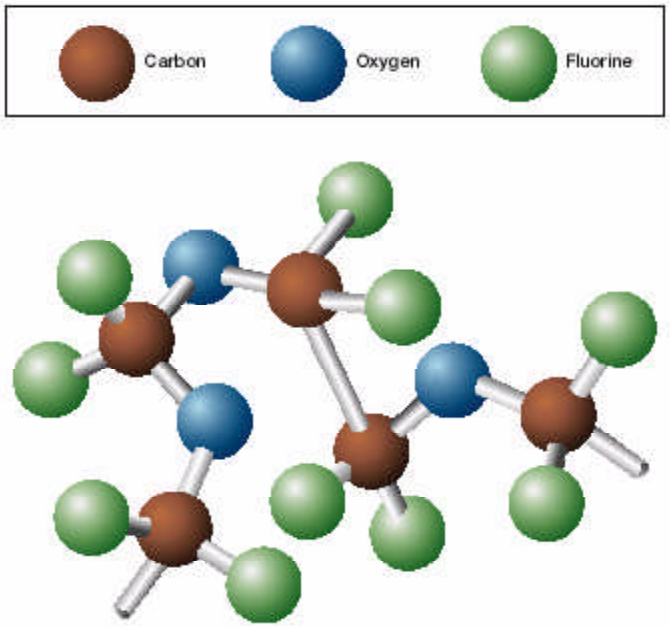
Computational Chemistry and Lubrication

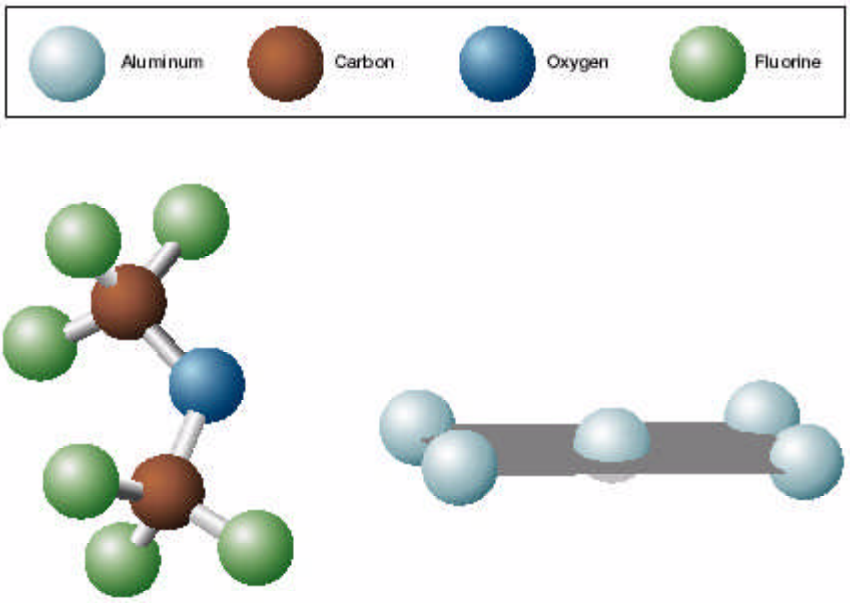


Chemical composition of one typical commercial perfluorinated polyalkyl ether lubricant. Molecular weight, 10,000 to 50,000.

Members of NASA Lewis Research Center's Tribology and Surface Science Branch are applying high-level computational chemistry techniques to the development of new lubrication systems for space applications and for future advanced aircraft engines. The next generation of gas turbine engines will require a liquid lubricant to function at temperatures in excess of 350 °C in oxidizing environments. Conventional hydrocarbon-based lubricants are incapable of operating in these extreme environments, but a class of compounds known as the perfluoropolyether (PFAE) liquids (see the preceding illustration) shows promise for such applications. These commercially available products are already being used as lubricants in conditions where low vapor pressure and chemical stability are crucial, such as in satellite bearings and composite disk platters. At higher temperatures, however, these compounds undergo a decomposition process that is assisted (catalyzed) by metal and metal oxide bearing surfaces. This decomposition process severely limits the applicability of PFAE's at higher temperatures. A great deal of laboratory experimentation has revealed that the extent of fluid degradation depends on the chemical properties of the bearing surface materials. Lubrication engineers would like to understand the chemical breakdown mechanism to design a less vulnerable PFAE or to develop a chemical additive to block this degradation.

The chemical reactions that take place between the PFAE chain and the surface are being studied successfully with quantum chemical techniques in which all "experiments" are done on the computer. A cluster of metal atoms representing the surface is approached by

a molecule of lubricant, and the detailed chemistry that takes place is accurately computed (see the next illustration). By adjusting the relative orientation of the approaching ether and the surface, and by changing the chemical makeup of the surface cluster, one can begin to understand what factors influence the lubricant decomposition. This understanding will help us design a surface-lubricant-additive combination that is stable at high temperatures.



Nondissociative binding site (edge site) of five-atom Al cluster/perfluorodimethyl ether complex. Ether oxygen is directed toward the aluminum atoms.

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